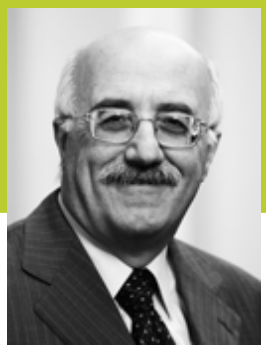
2012-13

Hirschfelder Lectures in Theoretical Chemistry



Professor Michele Parrinello, ETH-Zürich

Atomistic computer simulations: past, present and future

Monday, October 1 2:00 p.m. Room 1315 Chemistry

The rapid development of computer technology and new efficient algorithms have had deep impact on science. Of particular significance has been the emergence of realistic atomistic simulation. These calculations provide precious insight, replace difficult experiments and predict new phenomenon. Yet in spite of remarkable progress much remains to be done to widen the scope of atomistic simulation, especially in the fields of nanotechnology and biosciences. This requires extending the time and length of scales the system studied. Even more challenging is the need to find appropriate tools to describe and tame the complexity of the systems of current interest.

Molecular dynamics of nucleation and growth of crystals from solution

Tuesday, October 2 11:00 a.m. Room 1315 Chemistry

Nucleation and growth of crystals from solution is a phenomenon of great practical relevance. Yet its study is rather challenging both experimentally and theoretically. Computer simulations could be of great help; however they are rather difficult. To this effect we have developed a number of methods that can help in overcoming many of the difficulties. We shall present results on the growth of urea from aqueous solutions in the presence and the absence of additives. We show how additives, in particular biuret, can control the shape of the growing crystal. We also show how the nucleation from saturated water solution of the humble NaCl hides some remarkable surprises.

Proteins in Motion

Wednesday, October 3 2:00 p.m. Room 1315 Chemistry

Structural biology has played a major role in our understanding of the way proteins operate and work. Still, the knowledge of the structure alone offers a limited insight into protein dynamics. In this respect molecular dynamics can play a major role in complementing experiments and in getting precious dynamical information. However biomolecules are characterized by complex and rough landscapes and their functionality relies in a delicate balance between enthalpy and entropy. Accurate sampling of the phase space is therefore necessary but the limited time scale that is accessible with modern commercially available computers hampers it. Accelerated sampling techniques are therefore necessary. Here we discuss metadynamics which allows efficient sampling and permits an accurate reconstruction of the free energy landscape. We shall show that phenomena that take place on the time scale of milliseconds can be accurately sampled and subtle phenomena like allosteric interaction microscopically understood.